

# GOALI/FRG: Structural Properties of Alumina and Adsorbed Metal Particles

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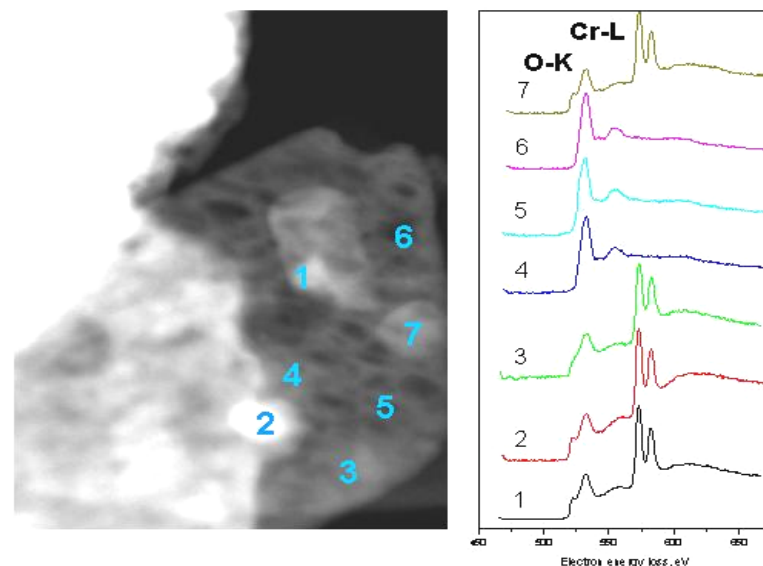
Some transition alumina ( $\text{Al}_2\text{O}_3$ ) polytypes are widely used as a catalytic support (on which catalyst metal particles are dispersed). We combined theoretical and experimental tools to obtain a comprehensive microscopic account of the structural stabilization and catalytic behavior of metal particles (Cr, La, Rh, Pd, Pt, etc.) on the alumina surfaces. The interaction between a dopant and the surface may be characterized by the change in the sample coloration (caused by splitting of the d-band of transition metal in the crystalline field). In some Cr doped samples, we observed  $\text{Cr}_2\text{O}_3$  accumulation at the surface. However, both theory and experiment show that the catalytic activity of the alumina is related to a dilute distribution of small  $\text{CrO}_x$  clusters rather than to crystalline  $\text{Cr}_2\text{O}_3$  precipitates.

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Change in coloration in different Cr-doped transition aluminas



EELS spectra Cr-doped  $\gamma\text{-Al}_2\text{O}_3$  taken from various places on a surface. Brighter regions on a Z-contrast image show accumulation of  $\text{Cr}_2\text{O}_3$ .

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## **Education, training, and development:**

Two undergraduates (John Ash and Ari B. Silver), one graduate student (Ying Hu), and three postdocs (Albina Borisevich, Shuhui Cai, and Sanwu Wang) contributed to this work. Prof. Karl Sohlberg (co-PI) got a prestigious “DuPont Young Professor” award for his work on computational materials science (including his work on transition aluminas and their phase transformations). The universities benefited from visits of the industrial collaborators and their presentations for the materials science/material physics community. A very productive collaboration with scientists from the Russian Academy of Sciences (Moscow and Novosibirsk) has been established.

## **Other specific products:**

This project has stimulated the upgrade of the existing scanning transmission electron microscopy (STEM) facility at Oak Ridge National Laboratory. At present, the STEM has the world's highest resolution for Z-contrast imaging. After upgrading (in the fall of 2003) this resolution was enhanced to about 0.6 - 0.7 Å for both Z-contrast imaging and EELS. The smaller beam size provides greatly improved signal to noise ratio for single atoms and crystals. This facilitates the direct imaging of dopant and impurity sites both on the alumina surface and in the bulk. A new facility, the Advanced Materials Characterization Facility is due to be constructed in the near future to house these upgraded instruments.